

Gauge Potential Formulations of the Spin Hall Effect in Graphene

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Abstract

Two different gauge potential methods are engaged to calculate explicitly the spin Hall conductivity in graphene. The graphene Hamiltonian with spin-orbit interaction is expressed in terms of kinematic momenta by introducing a gauge potential. A formulation of the spin Hall conductivity is established by requiring that the time evolution of this kinematic momentum vector vanishes. We then calculated the conductivity employing the Berry gauge fields. We show that both of the gauge fields can be deduced from the pure gauge field arising from the Foldy-Wouthuysen transformations.

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1 Introduction

For low energies and at the Dirac points where conduction and valance bands meet, graphene is described by some copies of the two-dimensional massless, free Dirac Hamiltonian after substituting the Fermi velocity v_F for the velocity of light c [1]. Mass gaps can be generated by taking into account spin-orbit interactions. One of the interesting features of this Dirac-like theory is the accomplishment of the spin Hall effect in graphene[2]. It is based on the observation that within this Dirac-like theory the quantum Hall effect occurs in the absence of external magnetic fields[3]. This discovery of Kane and Mele (KM)[2] had far reaching consequences like a new phenomena called topological insulators (see [4] for a complete list of references). We would like to consider the Dirac-like Hamiltonian of KM and calculate the spin Hall conductivity in graphene directly using quantum mechanical and semiclassical methods.

We will present two different but somehow related approaches. The first method relies on the observation that the Hamiltonian proposed by KM can be rephrased by defining a non-Abelian gauge potential. We will deal mainly with the spin-orbit interaction which preserves spin. When the Hamiltonian is expressed in terms of a gauge potential one can introduce the related kinematic momentum vector and define its time evolution which can be conceived as the quantum mechanical analogue of the force. In the case of the Hall effect this is the Lorentz force. One may provide a method of calculating the Hall conductivity through the configurations obtained by requiring that the Lorentz force vanishes which can be generalized to the integer quantum Hall effect. We will show that acquainted with the gauge potential it is possible to derive explicitly the spin Hall conductivity in graphene imitating this formulation. It is in accord with the result of KM.

The Foldy-Wouthuysen transformations of the two-dimensional massive Dirac Hamiltonian can be employed to define a non-Abelian gauge field[5]. Because of being pure gauge field it leads to a vanishing field strength. However, in the adiabatic limit it generates the Abelian Berry gauge potential[6]. Examining the semiclassical equations of motion of electrons in the presence of Berry gauge fields, one can show that the Hall conductivity is related to the Berry curvature. We generalize this formulation to the Dirac-like Hamiltonian of KM and show explicitly that spin Hall conductivity can be written in terms of the Berry phases. On the other hand we will show that the gauge potential of the KM Hamiltonian which is furnished in the first method can be deduced from this non-Abelian gauge field in the limit of vanishing momenta.

The method of calculating the Hall conductivity through the configurations defined by the requirement that the time evolution of the canonical momentum vector vanishes is presented in Section 2. In Section 3 we first express the KM Hamiltonian in terms of a vector field. We then imitate the formulation of Section 2 to derive the spin Hall effect conductivity in graphene by taking into account only the spin conserving spin-orbit interaction. Section 4 is devoted to the calculation of the spin Hall effect in graphene in terms of the Berry phases. In the last section we discuss the relation between these two different gauge fields and comment on whether the other possible interaction terms can be treated similarly.

2 Integer quantum Hall effect

To illustrate the formalism which we will adopt to calculate the spin Hall conductivity in graphene we first would like to discuss the integer quantum Hall effect. Hall effect is a phenomena which occurs when electrons are constrained to move in a two-dimensional sample which is subjected to the uniform, perpendicular magnetic field B . Because of the Lorentz force the charge carriers will

move to one edge of the sample creating a potential difference between the two edges. By applying the in-plane, constant electric field \mathbf{E} one can balance this potential difference thus the electrons will move through the sample without deflection. Considering the velocity of the electrons in this system one can find the Hall current and derive the Hall conductivity[7]. It is possible to carry this approach into quantum mechanics and obtain the integer quantum Hall effect. To this aim let us introduce the kinematic momenta $\pi_i = p_i - a_i$ associated with the electromagnetic vector potential components $a_i = (eB/2c)\epsilon_{ij}r_j$; $i, j = 1, 2$, and consider the Hamiltonian

$$H_B = \frac{\boldsymbol{\pi}^2}{2m} - e\mathbf{E} \cdot \mathbf{r}. \quad (2.1)$$

The commutation relations obeyed by the kinematic momentum and position operators are

$$[r_i, \pi_j] = i\hbar\delta_{ij}, [r_i, r_j] = 0, [\pi_i, \pi_j] = i\hbar f_{ij},$$

where $f_{ij} = \partial a_j / \partial r_i - \partial a_i / \partial r_j$ is the electromagnetic field strength with the nonvanishing components

$$f_{12} = -f_{21} = \frac{e}{c}B.$$

The Heisenberg equations of motion following from the Hamiltonian (2.1) are

$$\dot{r}_j = \frac{\pi_j}{m}, \quad (2.2)$$

$$\dot{\pi}_i = eE_i + f_{ij}\dot{r}_j. \quad (2.3)$$

Obviously, the eigenvalues of these operators correspond to the velocity of charge carriers and the electromagnetic force acting on them, respectively. Thus quantum mechanically demanding that the electrons do not be deflected by the electromagnetic force, is equivalent to consider the states $\psi_H(\mathbf{r})$ satisfying

$$\dot{\boldsymbol{\pi}}\psi_H(\mathbf{r}) = 0. \quad (2.4)$$

One can observe that nontrivial $\psi_H(\mathbf{r})$ exists. This ensures that we can consider the subspace where (2.4) is satisfied and solve them to obtain the velocities of charge carriers which are not deflected as

$$v_i = \frac{c}{B}\epsilon_{ij}E_j.$$

Although we do not indicate explicitly these are the values of the “velocity operators” (2.2) in the subspace where the conditions (2.4) are fulfilled. Plugging these into the definition of the electrical current

$$\mathbf{j} = -e\kappa\mathbf{v}$$

where κ is the concentration of charge carriers, yields

$$j_i = \sigma_H\epsilon_{ij}E_j.$$

Thus the Hall conductivity is obtained as

$$\sigma_H = -\frac{ec\kappa}{B}. \quad (2.5)$$

We should also specify κ . The eigenstates of the Hamiltonian (2.1) for $\mathbf{E} = 0$, which describes the electrons moving on the plane in the presence of the perpendicular, constant magnetic field B are known as Landau levels. They correspond to the eigenvalues

$$E_n = \hbar\omega_c(n + \frac{1}{2}); \quad n = 1, 2, \dots,$$

where $\omega_c = \frac{eB}{mc}$. The density of states of each Landau level can be calculated to be

$$\rho_L(E) = \frac{m}{2\pi\hbar^2}.$$

For the two-dimensional free electrons one finds the same density of states. One can attain the concentration of charge carriers between the the ground state E_0 and the Fermi level $E_F^{(L)}$ as

$$\kappa = \int_{E_0}^{E_F^{(L)}} \rho_L(E) dE = \frac{m}{2\pi\hbar^2} (E_F^{(L)} - E_0). \quad (2.6)$$

For Landau levels $E_0 = \frac{\hbar\omega_c}{2}$ and $E_F^{(L)} = \hbar\omega_c(N + \frac{1}{2})$ with N being the index of the highest filled Landau level, so that (2.6) yields

$$\kappa = \frac{eBN}{hc}. \quad (2.7)$$

Inserting (2.7) into (2.5) one obtains

$$\sigma_H = -\frac{e^2}{h}N,$$

which characterizes the integer quantum Hall effect.

3 A gauge field formulation of graphene

Graphene is the one atom thick material composed of carbon atoms which are situated at the corners of hexagons arranged as a honeycomb lattice. It is constructed as a superposition of two triangular sublattices which are designated as A and B . Its conduction and valance bands touch at two inequivalent Dirac points K and K' . Around these points, for low energies, the particles are described by the free, massless, two-dimensional Dirac-like Hamiltonian[1]

$$H_0 = v_F \boldsymbol{\alpha} \cdot \mathbf{p}, \quad (3.1)$$

where v_F is the effective velocity of electrons and

$$\boldsymbol{\alpha} \equiv (\sigma_x \tau_z, \sigma_y). \quad (3.2)$$

$\sigma_{x,y,z}$ are the Pauli matrices acting on the states of the sublattices A and B , in the representation where $\sigma_z = \text{diag}(1, -1)$. The other Pauli matrix $\tau_z = \text{diag}(1, -1)$ labels states at the Dirac points K and K' . One can also introduce the Pauli matrices $s_{x,y,z}$ to identify the spin of electrons with $s_z = \text{diag}(1, -1)$. We do not explicitly state neither the direct product between these spaces nor the unit matrices. In the presence of the uniform magnetic field B in z direction the spin-orbit interactions proposed in [2] yield the Hamiltonian

$$H^G = H_0 + \Delta_{SO} \sigma_z \tau_z s_z + \lambda_R (\sigma_x \tau_z s_y - \sigma_y s_x) - \frac{eB}{2} (y \sigma_x - x \sigma_y \tau_z). \quad (3.3)$$

To imitate the formalism of Section 2 we need to express the interaction Hamiltonian (3.3) by means of gauge fields. Obviously, the magnetic field term can be written in terms of an electromagnetic gauge field. However, the fully fledged interaction Hamiltonian can be written as

$$H^G = v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi}^G$$

by substituting \mathbf{p} in the free Hamiltonian (3.1) with the kinematic momentum vector

$$\boldsymbol{\Pi}^G = \mathbf{p} - \mathbf{A}^G,$$

by introducing the following gauge potential components

$$A_x^G = i \frac{\Delta_{SO}}{2v_F} \sigma_y s_z - \frac{\lambda_R}{v_F} s_y + \frac{eB}{2v_F} \tau_z y, \quad (3.4)$$

$$A_y^G = -i \frac{\Delta_{SO}}{2v_F} \sigma_x \tau_z s_z + \frac{\lambda_R}{v_F} s_x - \frac{eB}{2v_F} \tau_z x. \quad (3.5)$$

The last terms are the ordinary electromagnetic gauge fields in the symmetric gauge and the second terms can be read directly from (3.3). The first terms are unusual and they arise through the algebra of the Pauli matrices: $\sigma_x \sigma_y = i \sigma_z$.

The operators Π_i^G and r_i satisfy the commutation relations

$$[r_i, \Pi_j^G] = i \hbar \delta_{ij}, \quad [r_i, r_j] = 0, \quad [\Pi_i^G, \Pi_j^G] = i \hbar \epsilon_{ij} F_{xy}^G. \quad (3.6)$$

The field strength is defined as

$$F_{ij}^G = \frac{\partial A_j^G}{\partial r_i} - \frac{\partial A_i^G}{\partial r_j} - \frac{i}{\hbar} [A_i^G, A_j^G].$$

Thus, for the non-Abelian gauge field (3.4), (3.5), it takes the form $F_{ij}^G = \epsilon_{ij} F_{xy}^G$ with

$$F_{xy}^G = \frac{eB}{v_F} \tau_z - \frac{\Delta_{SO}^2}{2\hbar v_F^2} \sigma_z \tau_z + \frac{i \Delta_{SO} \lambda_R}{\hbar v_F^2} (\sigma_y s_y + \sigma_x \tau_z s_x) + \frac{2\lambda_R^2}{\hbar v_F^2} s_z. \quad (3.7)$$

3.1 Spin Hall effect in graphene

To discuss spin Hall effect we require that only the the spin-orbit term conserving the third component of spin is nonvanishing in (3.3). Hence, we deal with the Hamiltonian

$$H = H_0 + \Delta_{SO} \sigma_z \tau_z s_z, \quad (3.8)$$

which can be written as

$$H = v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi},$$

through the kinematic momenta $\boldsymbol{\Pi} = \mathbf{p} - \mathbf{A}$, where the gauge field \mathbf{A} is obtained from (3.4)-(3.5) by setting $B = 0$, $\lambda_R = 0$:

$$A_x = i \frac{\Delta_{SO}}{2v_F} \sigma_y s_z, \quad A_y = -i \frac{\Delta_{SO}}{2v_F} \sigma_x \tau_z s_z. \quad (3.9)$$

This is a vector potential taking values in the $SU(2)$ group generated by $\sigma_{x,y,z}$. The curvature corresponding to (3.9) is

$$F_{xy} = \frac{-i}{\hbar} [A_x, A_y] = -\frac{\Delta_{SO}^2}{2\hbar v_F^2} \sigma_z \tau_z.$$

We are now equipped with the whole machinery needed to discuss the spin Hall effect imitating the formulation of the Hall conductivity presented in Section 2. Considering the electrons in the external constant electric field \mathbf{E} described by

$$H_E = H - e\mathbf{E} \cdot \mathbf{r}, \quad (3.10)$$

we will derive the Heisenberg equations of motion and obtain the spin current by requiring that the time evolution of the kinematic momentum vector vanishes. The “velocity” and “force” operators obtained through the Heisenberg equations of motion $\dot{\mathbf{r}} = \frac{i}{\hbar}[H_E, \mathbf{r}]$ and $\dot{\mathbf{\Pi}} = \frac{i}{\hbar}[H_E, \mathbf{\Pi}]$ are

$$\dot{r}_i = (\dot{x}, \dot{y}) = (v_F \sigma_x \tau_z, v_F \sigma_y), \quad (3.11)$$

$$\dot{\Pi}_i = \frac{i\Delta_{SO}}{\hbar} \sigma_z \tau_z s_z \Pi_i - \frac{\Delta_{SO}^2}{2\hbar v_F^2} \epsilon_{ij} \dot{r}_j \sigma_z \tau_z + eE_i. \quad (3.12)$$

Then, we demand that the “force” vanishes:

$$\dot{\mathbf{\Pi}}\Psi(\mathbf{r}) = 0. \quad (3.13)$$

One can easily show that for all of the components of the spinor wave function $\Psi(\mathbf{r})$ the same differential equation follows from (3.13):

$$\Psi^T(\mathbf{r}) = f(\mathbf{r})(1, 1, 1, 1, 1, 1, 1, 1), \quad (3.14)$$

$$\left[\frac{\Delta_{SO}^2}{\hbar^2} p_i^2 + (eE_i)^2 + \frac{\Delta_{SO}^4}{\hbar^2 v_F^2} \right] f(\mathbf{r}) = 0, \quad (3.15)$$

where $i = 1, 2$ is not summed over. In the rest of this section we deal with operators taking values in the subspace spanned with the spinors (3.14) and (3.15), although we will not explicitly write. In fact in this subspace we can now solve (3.13) to obtain the velocities

$$\dot{r}_i = \frac{2iv_F^2}{\Delta_{SO}} \epsilon_{ij} \Pi_j s_z + \dot{r}_{Hi}, \quad (3.16)$$

where we separated the electric field dependent part as

$$\dot{r}_{Hi} = -\frac{2e\hbar v_F^2 \epsilon_{ij} E_j}{\Delta_{SO}^2} \sigma_z \tau_z. \quad (3.17)$$

We would like to calculate the spin Hall conductivity, therefore the relevant parts in the solution (3.16) are the terms proportional to the electrical field components (3.17). Let us label the velocity of spin up carriers by \dot{r}_{Hi}^{\uparrow} and the velocity of spin down carriers by $\dot{r}_{Hi}^{\downarrow}$. We can further determine the velocities of particles in the K and K' valleys corresponding to 1 and -1 eigenvalues of τ_z as

$$\dot{r}_{Hi}^{\uparrow+} = -\frac{2e\hbar v_F^2 \epsilon_{ij} E_j}{\Delta_{SO}^2} \sigma_z, \quad \dot{r}_{Hi}^{\uparrow-} = \frac{2e\hbar v_F^2 \epsilon_{ij} E_j}{\Delta_{SO}^2} \sigma_z, \quad (3.18)$$

$$\dot{r}_{Hi}^{\downarrow+} = -\frac{2e\hbar v_F^2 \epsilon_{ij} E_j}{\Delta_{SO}^2} \sigma_z, \quad \dot{r}_{Hi}^{\downarrow-} = \frac{2e\hbar v_F^2 \epsilon_{ij} E_j}{\Delta_{SO}^2} \sigma_z. \quad (3.19)$$

The Hall currents of the spin-up and spin-down electrons are defined as

$$\mathbf{j}_H^{\uparrow} = n^{\uparrow+} \dot{\mathbf{r}}_H^{\uparrow+} + n^{\uparrow-} \dot{\mathbf{r}}_H^{\uparrow-}, \quad (3.20)$$

$$\mathbf{j}_H^{\downarrow} = n^{\downarrow+} \dot{\mathbf{r}}_H^{\downarrow+} + n^{\downarrow-} \dot{\mathbf{r}}_H^{\downarrow-}, \quad (3.21)$$

where $n^{\uparrow+}, n^{\uparrow-}, n^{\downarrow+}, n^{\downarrow-}$ indicate concentrations of the related carriers, The Hall currents (3.20), (3.21) can be employed to define the spin Hall current as

$$\mathbf{j}_H^s = \frac{\hbar}{2}(\mathbf{j}_H^{\uparrow} - \mathbf{j}_H^{\downarrow}). \quad (3.22)$$

We need to determine the concentrations $n^{\uparrow+}, n^{\uparrow-}, n^{\downarrow+}, n^{\downarrow-}$. This will be elaborated inspecting the corresponding Hamiltonians. In fact, there are four different two-dimensional Hamiltonians stemming from (3.8):

$$H = \begin{pmatrix} H^{\uparrow+} & 0 & 0 & 0 \\ 0 & H^{\uparrow-} & 0 & 0 \\ 0 & 0 & H^{\downarrow+} & 0 \\ 0 & 0 & 0 & H^{\downarrow-} \end{pmatrix}.$$

These two-dimensional Hamiltonians corresponding to the \uparrow, \downarrow spin and the K, K' valley are

$$H^{\uparrow+} = v_F(\sigma_x p_x + \sigma_y p_y) + \Delta_{SO}\sigma_z, \quad H^{\uparrow-} = v_F(-\sigma_x p_x + \sigma_y p_y) - \Delta_{SO}\sigma_z, \quad (3.23)$$

$$H^{\downarrow+} = v_F(\sigma_x p_x + \sigma_y p_y) - \Delta_{SO}\sigma_z, \quad H^{\downarrow-} = v_F(-\sigma_x p_x + \sigma_y p_y) + \Delta_{SO}\sigma_z. \quad (3.24)$$

The effect of the spin-orbit term is to create a gap in the energy band structure of the Hamiltonians. In terms of the eigenvalues of the momenta $\hbar\mathbf{k}$, (3.23) and (3.24) yield the same energy distribution

$$E = \pm \sqrt{v_F^2 \hbar^2 k^2 + \Delta_{SO}^2}, \quad (3.25)$$

corresponding to particle and antiparticle (hole) states. We choose $\Delta_{SO} > 0$ and let the Fermi energy of graphene be in the gap by setting $\mathbf{k} = 0$. Identifying the concentration of particles and antiparticles (holes) by n_p and n_a , we obtain

$$n^{\uparrow+} = \begin{pmatrix} n_p & 0 \\ 0 & n_a \end{pmatrix}, \quad n^{\uparrow-} = \begin{pmatrix} n_a & 0 \\ 0 & n_p \end{pmatrix}, \quad (3.26)$$

$$n^{\downarrow+} = \begin{pmatrix} n_a & 0 \\ 0 & n_p \end{pmatrix}, \quad n^{\downarrow-} = \begin{pmatrix} n_p & 0 \\ 0 & n_a \end{pmatrix}. \quad (3.27)$$

The derivations of (3.26) and (3.27) are elaborated in Appendix A. Inserting the carrier concentrations (3.26) and (3.27) into the definition of the spin Hall current (3.22) one obtains

$$j_{Hi}^s = -\frac{2e\hbar^2 v_F^2}{\Delta_{SO}^2} n \varepsilon_{ij} E_j, \quad (3.28)$$

where $n \equiv n_p - n_a$. Now, n can be calculated using the density of states corresponding to the energy distribution (3.25) found as

$$\rho_E(E) = \int \frac{d^2 k'}{(2\pi)^2} \delta(E - E') = \frac{|E|}{2\pi v_F^2 \hbar^2}.$$

The edges of band gap lie at Δ_{SO} and $-\Delta_{SO}$, hence when we consider positive Fermi energy which lies in the gap, the number of states is derived as

$$n = \int_0^{\Delta_{SO}} \rho_E(E) dE = \frac{|\Delta_{SO}| \Delta_{SO}}{4\pi \hbar^2 v_F^2}. \quad (3.29)$$

Plugging (3.29) into (3.28) yields

$$j_{Hi}^S = -\frac{e}{2\pi}\varepsilon_{ij}E_j$$

and we obtain the spin Hall conductivity as

$$\sigma_H^S = -\frac{e}{2\pi}.$$

This is in accord with the results of [3, 2].

4 Spin Hall conductivity as Berry phase

Topological nature of the Hall effect is well exhibited in terms of Berry phases. The semiclassical equations of motion are altered drastically in the presence of Berry gauge fields (see [8] and the references therein). They yield an anomalous velocity term for electrons which leads to the anomalous Hall conductivity. In fact, ignoring spin of electrons the Hall conductivity can be written in terms of the Berry curvature F_B on the Fermi surface[9, 10] as (a complete list of references for the Berry phase effects in this context can be found in the recent review [11])

$$\sigma_H = -\frac{e^2}{\hbar} \int^{E_F} \frac{d^2p}{(2\pi\hbar)^2} F_B. \quad (4.1)$$

Considering the electrons with spin, a generalization of (4.1) to the spin Hall effect was discussed in [12]. Note that in this section \mathbf{p} is not a quantum operator but denotes the classical phase space variable. We deal with four different two-dimensional Dirac-like theories (3.23), (3.24), thus we should take into account the contributions arising from each of them separately. We adopt the formulation of [5] to derive the Berry gauge fields arising from each one of the two-dimensional Hamiltonians (3.23), (3.24). Therefore, we should start with giving the unitary Foldy-Wouthuysen transformations ($U^{\uparrow\uparrow}, U^{\uparrow-}, U^{\downarrow+}, U^{\downarrow-}$) corresponding to the Dirac-like Hamiltonians ($H^{\uparrow+}, H^{\uparrow-}, H^{\downarrow+}, H^{\downarrow-}$). We would like to present them in the unified notation:

$$U \equiv \text{diag}(U^{\uparrow\uparrow}, U^{\uparrow-}, U^{\downarrow+}, U^{\downarrow-}).$$

The unitary Foldy-Wouthuysen transformation U can be engaged to define the gauge field[13, 5]

$$\mathcal{A} \equiv \text{diag}(\mathcal{A}^{\uparrow\uparrow}, \mathcal{A}^{\uparrow-}, \mathcal{A}^{\downarrow+}, \mathcal{A}^{\downarrow-}) = i\hbar U(\mathbf{p}) \frac{\partial U^\dagger(\mathbf{p})}{\partial \mathbf{p}}.$$

Exploring the Dirac-like Hamiltonians (3.23), (3.24), we introduce the following Foldy-Wouthuysen transformation

$$U = \frac{1}{\sqrt{2E(E + \Delta_{SO})}} \begin{pmatrix} \sigma_z H^{\uparrow+} + E & 0 & 0 & 0 \\ 0 & -\sigma_z H^{\uparrow-} + E & 0 & 0 \\ 0 & 0 & -\sigma_z H^{\downarrow+} + E & 0 \\ 0 & 0 & 0 & \sigma_z H^{\downarrow-} + E \end{pmatrix}, \quad (4.2)$$

where E is the positive energy depending on \mathbf{p} as $E = \sqrt{v_F^2 \mathbf{p}^2 + \Delta_{SO}^2}$. Observe that (4.2) is defined to satisfy

$$U H U^\dagger = E \sigma_z \tau_z s_z. \quad (4.3)$$

One can study each entry of (4.2) as in [5] and show that they lead to the gauge potential

$$\mathcal{A} = \frac{i\hbar}{2E^2(E + \Delta_{SO})} [v_F E(E + \Delta_{SO}) \boldsymbol{\alpha} \sigma_z \tau_z s_z + v_F^3 \sigma_z \tau_z s_z (\boldsymbol{\alpha} \cdot \mathbf{p}) \mathbf{p} + v_F^2 E (\boldsymbol{\alpha} \cdot \mathbf{p}) \boldsymbol{\alpha} - v_F^2 \mathbf{p} E]. \quad (4.4)$$

Its components can be written explicitly as

$$\mathcal{A}_x = \frac{\hbar(v_F E(E + \Delta_{SO}) \sigma_y s_z - v_F^3 (\sigma_y p_x - \sigma_x \tau_z p_y) s_z p_x + v_F^2 E \sigma_z \tau_z p_y)}{2E^2(E + \Delta_{SO})}, \quad (4.5)$$

$$\mathcal{A}_y = \frac{\hbar(-v_F E(E + \Delta_{SO}) \sigma_x \tau_z s_z - v_F^3 (\sigma_y p_x - \sigma_x \tau_z p_y) s_z p_y - v_F^2 E \sigma_z \tau_z p_x)}{2E^2(E + \Delta_{SO})}. \quad (4.6)$$

Because of being a pure gauge potential the field strength of (4.4) vanishes. However, one can consider the adiabatic approximation by projecting on the positive energy states:

$$\mathcal{A}^B \equiv P \mathcal{A} P. \quad (4.7)$$

By inspecting the positive eigenvalues of the (4.3) one can deduce that the projection operator P is

$$P \equiv \text{diag}(P_+^\uparrow, P_-^\uparrow, P_+^\downarrow, P_-^\downarrow) = \text{diag}(1, 0, 0, 1, 0, 1, 1, 0).$$

It should be noted that when projected on positive energy states only the last terms in (4.5) and (4.6) make nonvanishing contributions, so that the Abelian Berry gauge field is

$$\mathcal{A}_i^B = \frac{\hbar v_F^2}{2E(E + \Delta_{SO})} \epsilon_{ij} p_j \mathbf{1}_\tau s_z, \quad (4.8)$$

where the unit matrix $\mathbf{1}_\tau$ in the τ_z space is exhibited explicitly. It is worth emphasizing that in \mathcal{A} negative energy states are present, thus it possesses twice the matrix elements of \mathcal{A}^B . The nonvanishing component of the Berry curvature is given as

$$\mathcal{F} = \hbar \left(\frac{\partial \mathcal{A}_y^B}{\partial p_x} - \frac{\partial \mathcal{A}_x^B}{\partial p_y} \right) \equiv \text{diag}(\mathcal{F}_+^\uparrow, \mathcal{F}_-^\uparrow, \mathcal{F}_+^\downarrow, \mathcal{F}_-^\downarrow) = -\frac{\hbar^2 v_F^2 \Delta_{SO}}{2E^3} \mathbf{1}_\tau s_z. \quad (4.9)$$

We propose to generalize (4.1) to the spin Hall effect in graphene as

$$\sigma_H^S = -\frac{e}{2} \int_{-\infty}^{E_F^{(2)}} \frac{d^2 p}{(2\pi\hbar)^2} \left[(\mathcal{F}_+^\uparrow + \mathcal{F}_-^\uparrow) - (\mathcal{F}_+^\downarrow + \mathcal{F}_-^\downarrow) \right]. \quad (4.10)$$

$E_F^{(2)}$ denotes the highest energy level occupied in the two-dimensional system. Thus, inserting (4.9) into the definition (4.10) leads to

$$\begin{aligned} \sigma_H^S &= -\frac{e}{2} \int_{-\infty}^{E_F^{(2)}} \frac{d^2 p}{(2\pi\hbar)^2} \left(-\frac{2\hbar^2 v_F^2 \Delta_{SO}}{E^3} \right) \\ &= -\frac{e}{2\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \end{aligned} \quad (4.11)$$

This is in accord with the calculation of the spin Hall conductivity obtained by employing the Kubo formula which is presented in Appendix B.

We let the Fermi energy level of graphene lie in the gap, so that in (4.11) we set $E_F^{(2)} = \Delta_{SO}$ and obtain the spin Hall conductivity as

$$\sigma_H^S = -\frac{e}{2\pi}.$$

This is the value established in [2].

5 Discussions

The main difference between the gauge fields (3.9) and (4.8) is the fact that the latter is acquired from (4.4) in the adiabatic limit (4.7), thus it is within the particle bands of the two-dimensional Dirac-like theories, but the former one is non-Abelian which connects the particle and hole bands of the two-dimensional Dirac-like theories. However, also the non-Abelian gauge potential (3.9) can be obtained from the gauge field (4.4) in the vanishing momentum limit, up to a constant, as

$$\mathbf{A} = \left(\frac{i\Delta_{SO}^2}{\hbar v_F^2} \right) \mathcal{A}|_{\mathbf{p}=0}.$$

This limit corresponds to restrict the Fermi energy of graphene to lie in the gap. In fact, the calculation of the spin Hall conductivity presented in Section 3.1 is valid only for the Fermi energy lying in the gap. Therefore, although the calculation methods are different the gauge fields (3.9) and (4.8) result from the same gauge field (4.4) in two different limits.

The nonvanishing magnetic field $B \neq 0$ case can be studied similarly. However if we switch on the Rashba term $\lambda_R \neq 0$ in (3.3), the third component of spin is not conserved and in spite of the fact that we can introduce the gauge potential (3.4),(3.5), the related curvature (3.7) is not diagonal in the spin space. Hence the method of Section 3.1 is not anymore suitable to discuss the spin Hall effect.

Appendix A

Introducing the label $I = (\uparrow+, \uparrow-, \downarrow+, \downarrow-)$ corresponding to each of the two-dimensional Dirac-like Hamiltonians given in (3.23), (3.24), we define the number operators as

$$N^I = n_p |p^I\rangle \langle p^I| + n_a |a^I\rangle \langle a^I|, \quad (\text{A.1})$$

where $|p^I\rangle$ and $|a^I\rangle$ denote, respectively, the positive energy $E = \sqrt{v_F^2 \hbar^2 k^2 + \Delta_{SO}^2}$ and the negative energy $-E$ eigenspinors of the related Dirac-like Hamiltonians. For instance, let us consider the Hamiltonian for the spin up carriers in the K valley, $H^{\uparrow+}$, whose eigenspinors can be written in the chiral basis as

$$|p^{\uparrow+}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) e^{i\phi} \end{pmatrix}, \quad (\text{A.2})$$

$$|a^{\uparrow+}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2}) e^{i\phi} \end{pmatrix}, \quad (\text{A.3})$$

where $\cos \theta = \frac{\Delta_{SO}}{E}$ and $\tan \phi = \frac{k_y}{k_x}$. Plugging them into (A.1) leads to

$$N^{\uparrow+}(\mathbf{k}) = \begin{pmatrix} \frac{n_p+n_a}{2} + \frac{n_p-n_a}{2} \cos \theta & \frac{n_p-n_a}{2} e^{-i\phi} \sin \theta \\ \frac{n_p-n_a}{2} e^{i\phi} \sin \theta & \frac{n_p+n_a}{2} - \frac{n_p-n_a}{2} \cos \theta \end{pmatrix}. \quad (\text{A.4})$$

When the Fermi level of graphene is in the gap generated by the spin-orbit interaction we should set $\mathbf{k} = 0$, hence $\cos \theta = 1$ and (A.4) yields

$$N^{\uparrow+}(\mathbf{k} = 0) \equiv n^{\uparrow+} = \begin{pmatrix} n_p & 0 \\ 0 & n_a \end{pmatrix}.$$

In order to obtain the concentrations corresponding to the other Hamiltonians, we need to consider their eigenspinors. In fact, for the spin up carriers in the K' valley described with $H^{\uparrow-}$ the eigenspinors are

$$|p^{\uparrow-}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}, \quad (\text{A.5})$$

$$|a^{\uparrow-}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}. \quad (\text{A.6})$$

Inserting them into (A.1) and considering the vanishing momentum limit leads to

$$N^{\uparrow-}(\mathbf{k} = 0) = n^{\uparrow-},$$

where $n^{\uparrow-}$ is given in (3.26). Similarly, for the spin down carriers in the K valley, we can show that the eigenspinors of the Hamiltonian $H^{\downarrow+}$ are

$$|p^{\downarrow+}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2})e^{i\phi} \end{pmatrix}, \quad (\text{A.7})$$

$$|a^{\downarrow+}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2})e^{i\phi} \end{pmatrix}. \quad (\text{A.8})$$

Making use of them in (A.1) and setting $\mathbf{k} = 0$ yield the concentration number $n^{\downarrow+}$ given in (3.27):

$$N^{\downarrow+}(\mathbf{k} = 0) = n^{\downarrow+}.$$

The eigenspinors of the Hamiltonian $H^{\downarrow-}$ corresponding to the spin down carriers in the K' valley are

$$|p^{\downarrow-}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}, \quad (\text{A.9})$$

$$|a^{\downarrow-}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}. \quad (\text{A.10})$$

One can easily observe that they result in

$$N^{\downarrow-}(\mathbf{k} = 0) = n^{\downarrow-},$$

where $n^{\downarrow-}$ is given in (3.27).

Appendix B

Kubo formula corresponding to the Hamiltonians (3.23), (3.24) can be written in the notation of Appendix A as[14]

$$(\sigma_H^S)^I = \frac{e\hbar^2}{2} \int^{E_F^{(2)}} \frac{d^2k}{(2\pi)^2} \frac{2\text{Im} [\langle a^I | \dot{y} | p^I \rangle \langle p^I | \dot{x} | a^I \rangle]}{4E^2}, \quad (\text{B.1})$$

where \dot{x} , \dot{y} are the related velocity operators which can be read from (3.11) and

$$E_F^{(2)} = \sqrt{v_F^2 \hbar^2 k_F^2 + \Delta_{SO}^2}.$$

For $H^{\uparrow+}$ the velocity operators are $\dot{x} = v_F \sigma_x$, $\dot{y} = v_F \sigma_y$ and the eigenspinors $|p^{\uparrow+}\rangle$ and $|a^{\uparrow+}\rangle$ are given in (A.2) and (A.3). Employing them in (B.1) leads to[15]

$$(\sigma_H^S)^{\uparrow+} = -\frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \quad (\text{B.2})$$

For the spin up carriers in the K' valley, we set $\dot{x} = -v_F \sigma_x$, $\dot{y} = v_F \sigma_y$ and deal with the eigenspinors (A.5),(A.6). We obtain the same conductivity

$$(\sigma_H^S)^{\uparrow-} = -\frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \quad (\text{B.3})$$

The contributions arising from the spin down carriers in the K and K' valleys are also equal but differ in sign with the spin up contributions:

$$(\sigma_H^S)^{\downarrow+} = (\sigma_H^S)^{\downarrow-} = \frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \quad (\text{B.4})$$

To obtain the spin Hall conductivity we should take the difference of the spin up and spin down contributions as

$$\sigma_H^S = ((\sigma_H^S)^{\uparrow+} + (\sigma_H^S)^{\uparrow-}) - ((\sigma_H^S)^{\downarrow+} + (\sigma_H^S)^{\downarrow-}). \quad (\text{B.5})$$

Inserting (B.2), (B.3) and (B.4) into (B.5) leads to the spin Hall conductivity

$$\sigma_H^S = -\frac{e}{2\pi} \frac{\Delta_{SO}}{E_F^{(2)}}.$$

This is the same with the result obtained in terms of the Berry phase (4.11).

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